Invariant Perturbation Theory of Adiabatic Process

Jian-Lan Chen, Mei-sheng Zhao, Jian-da Wu and Yong-de Zhang
Department of Mordern Physics and Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, 230026, China

In this paper we present an invariant perturbation theory of adiabatic process according to the concepts of $U(1)$-invariant adiabatic orbit and $U(1)$-invariant adiabatic expansion. The probabilities of keeping the adiabatic orbit in the first-order and the second-order approximation are calculated, respectively. We also give a convenient sufficient condition.

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Quantum adiabatic theorem and adiabatic approximation are important contents in quantum mechanics [1, 2, 3, 4]. Since the establishment of the quantum adiabatic theorem it has been broadly applied both in theory and experiments. In the deep investigation into quantum adiabatic process a lot of important results have been obtained, for example, Landau-Zener Transition [5], Gell-Mann-Low theorem [6], Berry phase[7], holomony[8]. Recently, the content of quantum information and quantum computation has revived interest in quantum adiabatic theorem and adiabatic approximation [9, 10, 11, 12, 13, 14]. More recently, however, the consistency of the traditional adiabatic approximation condition has been doubted [15, 16] and some new adiabatic conditions are proposed [17, 18, 22], which have caused confusions. Then, it is important to find a proper and convenient condition under which the evolution of the system can be considered adiabatic.

This paper is aimed to propose a general invariant perturbation theory for the quantum adiabatic process in terms of the concepts of $U(1)$-invariant adiabatic orbit and $U(1)$-invariant adiabatic expansion. Then, the probabilities of keeping in adiabatic orbit are obtained in the first-order and the second-order approximation, respectively. At last, a new and convenient adiabatic condition is presented.

Firstly, we explain the invariant adiabatic basis and invariant adiabatic expansion [19] with time-dependent coefficients. Let us consider a time-dependent Hamiltonian $H(t)$ with the initial state $|m,0\rangle$ at time $t=0$, here m denotes the initial value of dimensionless quantum number set. We introduce a dimensionless time parameter $\tau = E_m(0)t/\hbar$ and a dimensionless Hamiltonian $h(\tau) = H(\tau)/E_m(0)$, $E_m(0)$ is the energy of the initial state. The time-dependent *Schrödinger* equation reads

$$\begin{aligned} i\frac{\partial|\Phi_m(\tau)\rangle}{\partial\tau} &= h(\tau)|\Phi_m(\tau)\rangle, \quad |\Phi_m(\tau)\rangle|_{\tau=0} = |m,0\rangle \\ |\Phi_m(\tau)\rangle &= Te^{-i\int_0^\tau h(\lambda)d\lambda}|m,0\rangle, \end{aligned} \tag{1}$$

here T is time-ordered operator.

Definition 1: A state $|\Phi_n(\tau)\rangle$, is a *dynamic evolution orbit* of system when the state $|\Phi_n(\tau)\rangle$ satisfies Eq.(1), describing an evolution orbit varying with time in the Hilbert space.

Furthermore, if we consider τ as a fixed parameter, we can always solve the following quasi-stationary state equation

$$h(\tau)|\varphi_n(\tau)\rangle = e_n(\tau)|\varphi_n(\tau)\rangle \tag{2}$$

then we will have the *adiabatic solution* or *adiabatic orbit* $|\varphi_n(\tau)\rangle$ and its corresponding eigenvalue $e_n(\tau) = E_n(\tau)/E_m(0)$.

Of course, although with the same initial state $|m,0\rangle$, the dynamic evolution orbit $|\Phi_m(\tau)\rangle$ does not coincide with the adiabatic orbit $|\varphi_m(\tau)\rangle$, or they are not even close to each other. Furthermore, because of the Hermitian of $h(\tau)$, all of these adiabatic orbits form a complete basis of the system.

We denote $\gamma_{nm}(\tau) \equiv i\langle\varphi_n(\lambda)\mid\dot{\varphi}_m(\lambda)\rangle$ and the dot means the differentiation with respect to time. An adiabatic orbit multiplied by an arbitrary time-dependent phase factor still describes the same adiabatic orbit.

Definition 2: The following adiabatic orbits

$$\left|\Phi_m^{adia}(\tau)\right\rangle = \exp\left\{-i\int_0^\tau [e_m(\lambda)-\gamma_{mm}(\tau)]d\lambda\right\}|\varphi_m(\tau)\rangle \tag{3}$$

are invariant, up to a time-dependent phase factor, under $U(1)$ time-dependent transformation of the adiabatic orbit

$$|\varphi_m(\tau)\rangle \to e^{if_m(\tau)}|\varphi_m(\tau)\rangle, \tag{4}$$

with $f_m(0)=0$. We define this adiabatic orbit with special choice of the time-dependent phase factor as $U(1)$ *invariant adiabatic basis* which keeps the initial value of dimensionless quantum number set m invariant.

Definition 3: If the $|\varphi_m(\tau)\rangle$ in Eq.(3) satisfies following conditions

$$\langle\varphi_n(\tau)\mid\dot{\varphi}_m(\tau)\rangle = 0, \quad \forall n\neq m \tag{5}$$

then $\left|\Phi_m^{adia}(\tau)\right\rangle$ is also the dynamic evolution solution of Eq.(1). We call this adiabatic orbit "*adiabatic evolution orbit*" of system.

Generally speaking, in an arbitrary evolution process, the dynamic evolution orbit $|\Phi_m(\tau)\rangle$ starting from the initial state $|m,0\rangle$ will change or even vibrate rapidly

among some adiabatic orbits. This case can be described by the probability P staying in the adiabatic obit

$$P_m(\tau) = \left|\left\langle \Phi_n^{adia}(\tau) \mid \Phi_m(\tau)\right\rangle\right|^2, \quad \forall n \neq m \tag{6}$$

Next our task is to find when the dynamic orbit is sufficiently close to the adiabatic orbit if Eq.(5) is not satisfied. Then, we will give the correct adiabatic approximation conditions.

In the $U(1) - invariant$ adiabatic basis the dynamic evolution orbit reads

$$|\Phi_m(\tau)\rangle = \sum_n c_n(\tau)|\Phi_n^{adia}(\tau)\rangle, \quad |\Phi_m(\tau)\rangle|_{\tau=0} = |m,0\rangle, \tag{7}$$

with initial conditions $c_m(0) = 1, c_n(0) = 0, \forall n \neq m$. The time-dependent coefficients $c_k(\tau)$ are governed by

$$\dot{c}_n(\tau) = i\sum_{k\neq n} M(\tau)_{nk} c_k(\tau), \tag{8}$$

where the diagonal elements of matrix $M(\tau)$ are zero and the non-diagonal elements of $M(\tau)$ read

$$\begin{aligned} M(\tau)_{k'k''} &= \langle \Phi_{k'}^{adia}(\tau)|i\frac{\partial}{\partial\tau}|\Phi_{k''}^{adia}\rangle, \quad \forall k' \neq k'' \\ &= e^{i\alpha_{k'k''}(\lambda)}\,|\gamma_{k'k''}(\tau),| \\ \alpha_{k'k''}(\tau) &= \int_0^\tau d\eta\,(e_{k'}(\eta) - e_{k''}(\eta)) + \xi_{k'k''}(\eta), \end{aligned} \tag{9}$$

here $\xi_{mn}(\tau) \equiv \int_0^\tau d\eta\,(\gamma_{nn}(\eta) - \gamma_{mm}(\eta)) + \arg\gamma_{mn}(\tau)$. $\Delta_{mn} = \dot{\xi}_{mn}$ is referred as *geometric potential* of this system. And for *geometric potential* one can obtain further detailed analysis and application in our other papers [20].

Then we can get the expanding coefficients with initial conditions $\vec{C}(0)\,(c_m(0) = 1, c_k(0) = 0, \forall k \neq m)$

$$\vec{C}(\tau) = \left(T\exp\left[i\int_0^\tau M(\lambda)d\lambda\right]\right)\vec{C}(0). \tag{10}$$

The element of Eq.(10) is

$$c_k(\tau) = \left(T\exp\left[i\int_0^\tau M(\lambda)d\lambda\right]\right)_{km}. \tag{11}$$

Apparently, Eq.(11) shows that the dynamic evolution is just an adiabatic evolution if Eq.(5) is satisfied. In addition, since $M(\tau)$ is Hermitian, the probability of the evolution is conservative, that is

$$|c_m(\tau)|^2 + \sum_k |c_k(\tau)|^2 = 1, \tag{12}$$

which shows the time-dependent system considered is not a dissipative system.

Secondly, we try to get the probability $P_m(\tau)$ of keeping in adiabatic orbit $|\phi_m(\tau)\rangle$. In the time-dependent dynamic evolution process, the probability of keeping in the adiabatic orbit $|\Phi_m^{adia}(\tau)\rangle$, i.e., keeping the dimensionless quantum numbers invariant, is

$$P_m(\tau) = |c_m(\tau)|^2 = \left|\left(T\exp\left[i\int_0^\tau M(\lambda)\right]\right)_{mm}\right|^2, \tag{13}$$

Then adiabatic approximation requires

$$P_m(\tau) \to 1, \tag{14}$$

It means that the transition probability from dynamic evolution orbit to any other adiabatic orbits can be neglected.

We can get the analytical expression of $P_m(\tau)$ using the approach of coefficients ratio. Integrate Eq.(8) and get

$$c_n(\tau) = \prod_{k\neq n} \exp\left[i\int_o^\tau M(\lambda)_{nk}\frac{c_k(\tau)}{c_m(\tau)}\right] \quad \forall n. \tag{15}$$

Obviously, this equation set can be solved by the iterative method. Consider Eq.(11) we can get the probability of remaining in $|\Phi_m^{adia}(\tau)\rangle$ from Eq.(15)

$$P_m(\tau) = \prod_{k\neq m}\left|\exp\left\{i\int_0^\tau d\lambda \frac{\left\{T\exp\left[i\int_0^\lambda d\eta M(\eta)\right]\right\}_{km}}{\left\{T\exp\left[i\int_0^\lambda d\eta M(\eta)\right]\right\}_{mm}} M(\lambda)_{mk}\right\}\right|^2. \tag{16}$$

From Eq.(16) we can also obtain a necessary and sufficient condition in a compact form

$$\mathrm{Re}\left\{ i\sum_{k\neq m}\int_0^\tau d\lambda \frac{\left(T\exp\left[i\int_0^\lambda d\eta\, M\left(\eta\right)\right]\right)_{km}}{\left(T\exp\left[i\int_0^\lambda d\eta\, M\left(\eta\right)\right]\right)_{mm}} M_{mk}\left(\lambda\right)\right\}\to 0. \tag{17}$$

Thirdly, we give various approximate approaches to calculate the probability.
1, According to Eq.(12) the first-order approximation of $P_m(\tau)$ is

$$P_m(\tau)\cong 1-\sum_{k\neq m}\left|\int_0^\tau d\lambda\langle\Phi_k^{adi}(\lambda)|\dot{\Phi}_m^{adi}(\lambda)\rangle\right|. \tag{18}$$

Then the necessary and sufficient conditions can be described as

$$\left|\int_0^\tau d\lambda\langle\Phi_k^{adi}(\lambda)|\dot{\Phi}_m^{adi}(\lambda)\rangle\right|^2\to 0,\quad \forall k\neq m. \tag{19}$$

Eq.(19) is of abundant contents which has been discussed in another paper [19]. Later we will obtain a convenient adiabatic condition from Eq.(19).
2, From Eq.(11) the second-order approximation of $P_m(\tau)$ is

$$P_m(\tau)\cong\left|\left(1-\int_0^\tau d\lambda_1\int_0^{\lambda_1}d\lambda_2 M\left(\lambda_1\right)M\left(\lambda_2\right)\right)_{mm}\right|^2. \tag{20}$$

because the first-order term of Eq.(11) is zero. The adiabatic approximate reads

$$\left|\sum_{k\neq m}\int_0^\tau d\lambda_1\int_0^{\lambda_1}d\lambda_2 M_{mk}\left(\lambda_1\right)M_{km}\left(\lambda_2\right)\right|^2\to 0. \tag{21}$$

3, the first-order of the coefficients ratio is. $c_k(\tau)$, $c_m(\tau)$ are all approximated in the first-order with $c_m(\tau)\cong 1$

$$\frac{c_k(\tau)}{c_m(\tau)}\cong i\int_0^\tau d\eta M_{km}(\eta). \tag{22}$$

We substitute Eq.(22) into Eq.(17)

$$\mathrm{Re}\left\{-\sum_{k\neq m}\int_0^\tau d\lambda M_{mk}\left(\lambda\right)\int_0^\lambda d\eta\, M_{km}\left(\eta\right)\right\}\to 0. \tag{23}$$

It should be pointed out that this method can only be applied to the situation without reversion of quantum state which can not be treated as adiabatic process with $c_m(\tau')=0$

Fourthly, as application of adiabatic invariant perturbation theory we consider a spin-1/2 charged particle in magnetic field. Eq.(19) can be rewritten as

$$\left|\int_0^\tau d\lambda M_{km}\right|^2=\left|\int_0^\tau d\lambda e^{i\alpha(\lambda)}|\gamma_{km}|\right|^2\to 0,\quad \forall k\neq m \tag{24}$$

Now we suppose $\ddot{\alpha}(\tau)=0$, then $\alpha(\tau)$ can be linearly expanded

$$e^{i\alpha(\tau)}=e^{i(\alpha_0+\Omega_0\tau)}. \tag{25}$$

where α_0, Ω_0 are constants. $|\gamma_{km}\left(\lambda\right)|$ is a periodic function can be expanded in Fourier series

$$\begin{aligned}\left|\int_0^\tau d\lambda e^{i\alpha(\lambda)}\left|\gamma_{km}\left(\lambda\right)\right|\right|^2 &= \left|\int_0^\tau d\lambda e^{i\Omega_0\lambda}\sum_l\Gamma_l^{(km)}e^{i\Omega_{km.l}\lambda}\right|^2\\ &= \left|\sum_l\frac{\Gamma_l^{(km)}}{(\Omega_0+\Omega_{km,l})}\right|^2.\end{aligned} \tag{26}$$

The adiabatic approximate condition reads

$$\left|\frac{\Gamma_l^{(km)}}{(\Omega_0+\Omega_{km,l})}\right|\ll 1,\quad \ddot{\alpha}(\tau)=0, \tag{27}$$

which is a convenient sufficient conditions [21]. In fact, $\ddot{\alpha}(\tau)=0$ is a physical requirement. For this kind of Hamiltonian [22]

$$H_V(t)=e^{-itV}He^{itV}, \tag{28}$$

where V and $H=\sum_n E_n|E_n\rangle\langle E_n|$ are two arbitrary time-independent Hamiltonian with $\{E_n,|E_n\rangle\}$ being the eigensystem of H. The quasi-stationary state of $H_V(t)$ is $e^{-itV}|E_n\rangle$. The adiabatic orbit reads

$$|\Phi_m^{adi}(\tau)\rangle=e^{-iE_m\tau+i\langle E_m|V|E_m\rangle\tau}e^{-itV}|E_n\rangle. \tag{29}$$

Then we get the elements of the matrix M

$$\begin{aligned}M_{nm} &= \langle\Phi_n^{adi}(\tau)|\dot{\Phi}_m^{adi}(\tau)\rangle\\ &= e^{-i(E_m-E_n)\tau+i\langle E_m|V|E_m\rangle\tau-i\langle E_n|V|E_n\rangle\tau}\langle E_n|V|E_m\rangle.\end{aligned} \tag{30}$$

The terms about τ in the exponent are all linear, which means $\ddot{\alpha}=0$ is satisfied. Therefore, we can prove concisely that the adiabatic condition Eq.(27) is sufficient for this kind of Hamiltonian. Next we will explain our above adiabatic condition Eq.(27) with model in [16]. For system a, the adiabatic approximate conditions is $\left|\frac{\omega\sin\theta}{\omega_0+\omega\cos\theta}\right|\ll 1$, under this condition the probability of remaining in adiabatic orbit is $P_m=1-\frac{\omega^2\sin^2\theta}{\tilde{\omega}^2}\sin^2\frac{\tilde{\omega}t}{2}\to 1$; For system b, the adiabatic approximate conditions is $|\tan\theta|\ll 1$, under this condition the probability of remaining in adiabatic orbit is $P_m=1-\sin^2\theta\sin^2\frac{\omega t}{2}\to 1$. It is not difficult to see that

the adiabatic conditions for system a and system b are different, then the inconsistency showed by this example does not exist when applying our condition. The trivial and special example of our condition with constant geometric potential and energy gap is proved in [18]. Of course, our condition with time-dependent geometric potential is more natural and general.

In conclusion, we present the invariant perturbation theory based on the concepts of invariant adiabatic orbit and expansion stated in our paper. The probability of keeping int the adiabatic orbit is given. Furthermore, we give an convenient adiabatic approximation condition which is more convenient to apply than the general sufficient showed in [16]. The derivation of our condition is more concise and general than [22]. The result is that we can obtain the approximate dynamic solution in perturbation theory by using the corresponding quasi-stationary equations and energy for nondissipative and smooth time-dependent process.

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